



	Experiment title: Structure-aided drug design. <i>BAG: Uppsala (II)</i>	Experiment number: LS-1665 unge
Beamline: ID14-4	Date of experiment: from: 29 April 2000 to: 30 April 2000	Date of report: 29 Aug 2001
Shifts: 3	Local contact(s): Dr. Julien LESCAR (e-mail: lescar@esrf.fr)	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): * Torsten Unge, Uppsala University, torsten@alpha2.bmc.uu.se * Seved Lövgren, Uppsala University, seved@alpha2.bmc.uu.se		

Report:

A data set was collected of HIV-1 protease in complex with the inhibitor bea450. Totally 200 images of 1 degree rotation were collected from unfrozen crystals. Data to 2.0 Å were obtained with a completeness of 99 %. The linear R-fac was for all reflexions 17.7%. The structure was refined to R value of 0.217 and Rfree of 0.24.4 The structure is used for the further development of these inhibitors.

A data set was collected of HIV-1 protease in complex with the inhibitor bea457. Totally 150 images of 1 degree rotation were collected from unfrozen crystals. Data to 1.9 Å were obtained with a completeness of 83 %. The linear R-fac was for all reflexions 11.4 %. The structure was refined to R value of 0.198 and Rfree of 0.225.

A data set was collected of HIV-1 reverse transcriptase drug resistant mutant K103N in complex with the inhibitor mst136. Totally 150 images of 0.5 degree rotation were collected

from unfrozen crystals. Data to 3.0 Å were obtained with a completeness of 98 %. The linear R-fac was for all reflexions 16 %. The structure was refined to R value of 0.250 and Rfree of 0.296.

A data set was collected of HIV-1 reverse transcriptase drup resistant mutant K103N in complex with the inhibitor efavirenz. Totally 100 images of 0.5 degree rotation were collected from unfrozen crystals. Data to 3.0 Å were obtained with a completeness of 88 %. The linear R-fac was for all reflexions 16.1 %. The structure was refined to R value of 0.227 and Rfree of 0.280.